

# 4-Bromobenzeneboronate, guaifenesin

**Inchi:** InChI=1S/C16H16BBrO4/c1-19-15-4-2-3-5-16(15)20-10-14-11-21-17(22-14)12-6-8-13(18)  
**InchiKey:** NNNJUMHAOJUKIP-UHFFFAOYSA-N  
**Formula:** C16H16BBrO4  
**SMILES:** COc1ccccc1OCC1COB(c2ccc(Br)cc2)O1  
**Mol. weight [g/mol]:** 363.01

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.15		Crippen Method
logp	2.647		Crippen Method
rinsol	2455.00		NIST Webbook
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## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R146731&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**rinsol:** Non-polar retention indices

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